## "Thermodynamic Analysis of Processes for Hydrogen Generation by Decomposition of Water" by John P. O'Connell Department of Chemical Engineering University of Virginia Charlottesville, VA 22904-4741

## A Set of Energy Education Modules for Chemical Engineering Sponsored by The Center for Energy Initiatives of The American Institute of Chemical Engineers Institute for Sustainability

## Module 4: A Simplified Multisection Process for Thermochemical Hydrogen

## Introduction

Module 1 of this series provides the foundation thermodynamic analysis of processes for energy effects and process constraints doule 2 provides experience with single-unit processes. Module 3 treats processes for the terminal decomposition of water for hydrogen manufacture from an overall point of view. ell present Module does an analysis of a water decomposition process involving 2 sections that exchange methane and methanol as well as heat. The objective is to gain experience in treating ycles and multiple sections involving reactions that can then be built on in Module 5 that analyzes the 3-section Sulfur-Iodine process.

We first repeat essential elements of ModuleFigure 4.1illustrates the concept for a steady-flow system, with inlet and outletestms at specified absolute temperaturepressures, P, and sets of molar or mass amounts for the componentification with energy that crosses the boundaries as "shaft workWs, and heatQ. Note that if a stream has both vapor and liquid, its specification must include the amounts of ponents in the phases. For pure components, this means specifying either P, the total flow,N, and the quality or fraction of the system that is vaporx. For mixtures, defining the state is mediaborate. The balance equations for steady flow processes are:

Figure 4.1. Steady Flow System for Applyi**M**gaterial, Energy, and Entropy Relations, Eqs. (4.1) and (4.2).

$$\sum_{i} N_{i}h_{i}(T_{i}, P_{i}, x_{i}) = N_{o}h_{o}(T_{o}, P_{o}, x_{o}) = W_{s} = Q_{b} = Q_{e} = 0$$

$$(4.1)$$

$$N_{i}s_{i}(T_{i}, P_{i}, x_{i}) = N_{i}s_{i}(T_{i}, P_{i}, x_{o}) = Q_{b} = Q_{b}$$

$${}_{i} N_{i} s_{i} (T_{i}, P_{i}, x_{i}) {}_{i} N_{o} s_{o} (T_{o}, P_{o}, x_{o}) {}_{b} {}^{\sim b} T_{b}$$

$$(4.2)$$

the reactions in the sections connects the **slool** these streams. This is not a necessary assumption, but significantly simplifies the analysis.

Figure IV.1. Simplified Schematic Diagram of Schulten Process for Thermochemical Decomposition of Water to Manufacture Hydrogen. Subscripts for speciAs-alveethanol,

Table 4.3 shows problem specifications deecomposing water by the Schulten process, with the streams and properties of Table IV.2  $\mathcal{B}_{net}$  313K, and  $T_{21}$  = 491 K

Table 4.3 Specific Problems for Case IB bld = Specified Italic = Solved. The Helium states are set at  $T_{i1}$